



RECEIVED  
OCT 21 2003  
TC 1700

IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

In re Application of TAKAOKI et al.

Serial No. : 09/739,802

Group Art Unit : 1754

Filed : December 20, 2000

Examiner : KUHAR, ANTHONY J.

For: CATALYST COMPONENT FOR ADDITION POLYMERIZATION, CATALYST  
FOR ADDITION POLYMERIZATION, AND PROCESS FOR PRODUCING  
ADDITION POLYMER

\* \* \* \* \*

DECLARATION UNDER 37 C.F.R. §1.132

Honorable Commissioner of Patents and Trademarks  
Washington, D.C. 20231

Sir:

I, Hiroshi KURIBAYASHI, a Japanese citizen residing at  
5-6-26, Souja, Ichihara-shi, Chiba, Japan,  
declare:

That I am one of inventors of the identified-application;

That I am familiar with the prosecution history of the  
identified-application; and

That the following calculations were conducted by me.

## 1. Purpose

To know whether or not the lowest energy level of unoccupied molecular orbital having the valence p-type atomic orbital of a zinc atom of tetraphenylporphyrinzinc chloride tetrakis(pentafluoroborate) or an iron atom of tetraphenylporphyriniron chloride tetrakis(pentafluoroborate) (wherein the coefficient represented by a linear combination is 0.4 or more) disclosed in EP 0 638 184 A1 cited in the Office Action mailed on July 16, 2003, is calculated to be 0.008 (atomic unit (Hartree)) or less by the calculation of density functional method (B3LYP/3-21G level).

## 2. Calculation

### Conditions for calculation

- (A) A program (software) used: Gaussian 98 (manufactured by Gaussian Inc.)
- (B) Calculation method: B3LYP
- (C) Basis Set: 3-21G (the program with built-in basis set)
- (D) Input structural data: As structural data(x, y and z coordinates), values optimized by MM2 program of CAChe system (manufactured by Fujitsu Limited) were used.

- (1) Calculation of orbital energy of molecular orbital of tetraphenylporphyrinzinc chloride

#### tetrakis(pentafluoroborate)

The calculation was carried out under which the charge was zero and the spin multiple degree was 1 in addition to the conditions (A) to (D) mentioned above.

As the calculation result, it was confirmed that the lowest energy level of unoccupied molecular orbital having the valence p-type atomic orbital of Zn as a main component (wherein the coefficient represented by a linear combination was 0.4 or more) was calculated to be 0.06394 atomic unit (Hartree).

#### 2. Calculation of orbital energy of molecular orbital of tetraphenylporphyriniron chloride tetrakis(pentafluoroborate)

The calculation was carried out under which the charge was zero and the spin multiple degree was 3 in addition to the conditions (A) to (D) mentioned above.

As the calculation result, it was confirmed that the lowest energy level of unoccupied molecular orbital having the valence p-type atomic orbital of Fe as a main component (wherein the coefficient represented by a linear combination was 0.4 or more) was calculated to be 0.05875 atomic unit (Hartree).

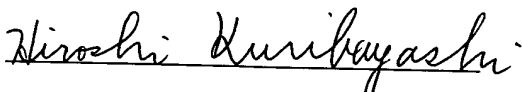
### **3. Conclusion**

The lowest energy level of unoccupied molecular orbital having the valence p-type atomic orbital of a zinc atom of tetraphenylporphyrin zinc chloride

tetrakis(pentafluoroborate) or an iron atom of  
tetraphenylporphyriniron chloride  
tetrakis(pentafluoroborate) is 0.06394 or 0.05875,  
respectively, and was not 0.008 or less. Therefore, these  
compounds are not included in the compounds specified in the  
claims of the above-identified application.

That I declare further that all statements made herein of  
my own knowledge are true and that all statements made on  
information and belief are believed to be true; and further  
that these statements were made with the knowledge that willful  
false statements and the like so made are punishable by fine  
or imprisonment, or both, under Section 1001 of Title 18 of  
the United States Code, and that such willful false statements  
may jeopardize the validity of the above identified application  
or patent issued thereon.

Signed this day 24th of September, 2003.

  
Hiroshi KURIBAYASHI